

Quantum diffusion in the Kronig-Penney model

Masahiro Kaminaga ^{*} Takuya Mine [†]

Received: date / Accepted: date

Abstract

In this paper we consider the 1D Schrödinger operator H with periodic point interactions. We show an $L^1 - L^\infty$ bound for the time evolution operator e^{-itH} restricted to each energy band with decay order $O(t^{-1/3})$ as $t \rightarrow \infty$, which comes from some kind of resonant state. The order $O(t^{-1/3})$ is optimal for our model. We also give an asymptotic bound for the coefficient in the high energy limit. For the proof, we give an asymptotic analysis for the band functions and the Bloch waves in the high energy limit. Especially we give the asymptotics for the inflection points in the graphs of band functions, which is crucial for the asymptotics of the coefficient in our estimate.

1 Introduction

The one-electron models of solids are based on the study of Schrödinger operator with periodic potential. There are a lot of studies on the periodic potential, in particular, for periodic point interactions, we can show the spectral set explicitly (Albeverio et. al. [2] is the best guide to this field for readers). Most fundamental case is the one-dimensional Schrödinger operator with periodic point interactions, called the *Kronig-Penney model* (see Kronig-Penney [10]), given by

$$H = -\frac{d^2}{dx^2} + V \sum_{j=-\infty}^{\infty} \delta(x - j) \quad \text{on } L^2(\mathbf{R}), \quad (1)$$

where V is a non-zero real constant, and $\delta(\cdot - j)$ is the Dirac delta measure at $j \in \mathbf{Z}$. The positive sign of V corresponds the repulsive interaction, while the negative one corresponds the attractive one. More precisely, H is the negative Laplacian with boundary conditions on integer points:

$$H = -\frac{d^2}{dx^2} \quad \text{on } \mathcal{D}, \quad (2)$$

^{*}Department of Electrical Engineering and Information Technology, Tohoku Gakuin University, Tagajo, 985-8537, JAPAN. Tel.: +81-22-368-7059 E-mail:kaminaga@mail.tohoku-gakuin.ac.jp

[†]Faculty of Arts and Sciences, Kyoto Institute of Technology, Matsugasaki, Kyoto, 606-8585, JAPAN. Tel: +81-75-724-7834 E-mail: mine@kit.ac.jp

where

$$\mathcal{D} = \{u \in H^1(\mathbf{R}) \cap H^2(\mathbf{R} \setminus \mathbf{Z}) : u'(j+) - u'(j-) = Vu(j), j \in \mathbf{Z}\}. \quad (3)$$

Here $u(j\pm) = \lim_{\epsilon \rightarrow +0} u(j \pm \epsilon)$ and $H^p(\Omega)$ is the usual Sobolev space of order p on the open set Ω . From Sobolev's embedding theorem $H^1(\mathbf{R}) \hookrightarrow C_b^0(\mathbf{R})$, every elements of \mathcal{D} are continuous (classical sense) and uniformly bounded functions. It is well-known that H is self-adjoint [4, 2] and is a model describing electrons on the quantum wire. The spectrum of this model is explicitly given by

$$\sigma(H) = \left\{ E \in \mathbf{R} : -2 \leq D(\sqrt{E}) \leq 2 \right\}, \quad (4)$$

where

$$D(k) = 2 \cos k + V \frac{\sin k}{k}.$$

$D(k)$ is so-called *discriminant* and $D(\sqrt{E})$ can be regarded as an entire function with respect to $E \in \mathbf{C}$. The spectrum $\sigma(H)$ of H consists of infinitely many closed intervals (spectral bands) and is purely absolutely continuous.

On the other hand, for the Schrödinger operator $H = -\Delta + V$ on \mathbf{R}^d with decaying potential V , the *dispersive estimate* for the Schrödinger time evolution operator e^{-itH} is stated as follows:

$$\begin{aligned} \|P_{ac} e^{-itH} u\|_{L^p(\mathbf{R}^d)} &\leq C |t|^{-d(\frac{1}{2}-\frac{1}{p})} \|u\|_{L^q(\mathbf{R}^d)}, \quad u \in L^2(\mathbf{R}^d) \cap L^q(\mathbf{R}^d) \\ (2 < p \leq \infty, 1/p + 1/q = 1), \end{aligned} \quad (5)$$

where P_{ac} denotes the spectral projection to the absolutely continuous subspace for H . The dispersive estimate is a quantitative representation of the diffusion phenomena in quantum mechanics, and is extensively studied recently, because of its usefulness in the theory of the non-linear Schrödinger operator (see e.g. Journé–Soffer–Sogge [11], Weder [18], Yajima [17], Mizutani [12], and references therein). The estimate (5) is also obtained in the case of the one-dimensional point interaction. Adami–Sacchetti [1] obtain (5) when V is one point δ potential, and so do Kovařík–Sacchetti [9] when V is the sum of δ potentials at two points. The motivation of the present paper is to obtain a similar estimate for our periodic model (1). Though this problem is quite fundamental, we could not find such kind of results in the literature, probably because the deduction of the result requires a detailed analysis of the band functions, as we shall see below.

Since the spectrum of the Schrödinger operator with periodic potential is absolutely continuous, one may expect some dispersion type estimate holds also in this case. However, there seems to be few results about the dispersive type estimate for the time evolution operator of the differential equation with periodic coefficients.¹ An example is the paper by Cuccagna [3], in which the Klein–Gordon equation

$$\begin{aligned} u_{tt} + Hu + \mu u &= 0, \quad H = -\frac{d^2}{dx^2} + P(x) \quad \text{on } \mathbf{R}, \\ u(0, x) &= 0, \quad u_t(0, x) = g(x) \end{aligned}$$

¹Some authors study the pointwise asymptotics for the integral kernel of the time evolution operator in the large time limit; see e.g. Korotyaev [8] and references therein. But we could not find the dispersive type estimate for the periodic Schrödinger operator itself in the literature.

is considered, where $P(x)$ is a smooth real-valued periodic function with period 1. Cuccagna proves the solution $u(t, x)$ satisfies

$$\|u(t, \cdot)\|_{L^\infty(\mathbf{R})} \leq C_\mu \langle t \rangle^{-1/3} \|g(\cdot)\|_{W^{1,1}(\mathbf{R})}, \quad \langle t \rangle = \sqrt{1+t^2} \quad (6)$$

for $\mu \in (0, \infty) \setminus D$, where D is some bounded discrete set. The peculiar power $-1/3$ comes from the following reason. The integral kernel for the time evolution operator is written as the sum of oscillatory integrals

$$K_{n,t}(x, y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-it(\lambda_n(\theta) - s\theta)} a_n(\theta, x', y') d\theta \quad (n = 1, 2, \dots), \quad (7)$$

where $x = [x] + x'$, $y = [y] + y'$, $[x], [y] \in \mathbf{Z}$, $x', y' \in (0, 1)$, and $s = ([x] - [y])/t$. The function $\lambda_n(\theta)$ is called the *band function* for the n -th band, which is a real-analytic function of θ with period 2π . In the large time limit $t \rightarrow \infty$, it is well-known that the main contribution of the oscillatory integral (7) comes from the part nearby the *stationary phase point* θ_s (the solution of $\lambda'_n(\theta) = s$), and the *stationary phase method* tells us the principal term in the asymptotic bound is a constant multiple of $|\lambda''_n(\theta_s)|^{-1/2} t^{-1/2}$ (see e.g. Stein [15, Chapter VIII] or Lemma 15 below). However, since $\lambda_n(\theta)$ is a periodic function, there exists a point θ_0 so that $\lambda''_n(\theta_0) = 0$. If the stationary phase point θ_s coincides with θ_0 , then the previous bound no longer makes sense. Instead, the stationary phase method concludes the principal term is a constant multiple of $|\lambda_n^{(3)}(\theta_0)|^{-1/3} t^{-1/3}$. Since the integral kernel of our operator has the same form as (7) (see (125) below), we expect a result similar to (6) also holds in our case.

Let us formulate our main result. Let H be the Hamiltonian for the Kronig-Penney model given in (2) and (3). As stated above, the spectrum of H has the band structure, that is,

$$\sigma(H) = \bigcup_{n=1}^{\infty} I_n,$$

where the n -th band I_n is a closed interval of finite length (for the precise definition, see (22) below). Our main result is as follows.

Theorem 1. *Let P_n be the spectral projection onto the n -th energy band I_n . Then, for sufficiently large n , there exist positive constants $C_{1,n}$ and $C_{2,n}$ such that*

$$\|P_n e^{-itH} u\|_{L^\infty} \leq (C_{1,n} \langle t \rangle^{-1/2} + C_{2,n} \langle t \rangle^{-1/3}) \|u\|_{L^1} \quad (8)$$

for any $u \in L^1(\mathbf{R})$ and any $t \in \mathbf{R}$, where $\langle t \rangle = \sqrt{1+t^2}$. The coefficients obey the bound

$$C_{1,n} = O(1), \quad C_{2,n} = O(n^{-1/9})$$

as $n \rightarrow \infty$.

The power $-1/2$ in the first term of the coefficient in (8) is the same as in (5) with $d = 1$ and $p = \infty$, since it comes from the states corresponding to the energy near the band center, which behaves like a free particle. This fact can be understood from the graph

of $\lambda = \lambda_n(\theta)$ (Figure 1).² The part of the graph corresponding to the band center is similar to the parabola $\lambda = \theta^2$ or its translation, which is the band function for the free Hamiltonian $H_0 = -d^2/dx^2$. On the other hand, the power $-1/3$ comes from part of the integral (7) given by

$$\tilde{K}_{n,t}(x, y) = \frac{1}{2\pi} \int_{J_n} e^{-it(\lambda_n(\theta) - s\theta)} a_n(\theta, x', y') d\theta, \quad (9)$$

where J_n is some open set including two solutions θ_0 to the equation $\lambda_n''(\theta) = 0$. Notice that $(\theta_0, \lambda_n(\theta_0))$ is an inflection point in the graph of $\lambda = \lambda_n(\theta)$; see Figure 1. The estimates for the coefficients are obtained from the lower bounds for the derivatives of $\lambda_n(\theta)$. Actually, we can choose J_n so that

$$\inf_{\theta \in [-\pi, \pi] \setminus J_n} |\lambda_n''(\theta)| \geq C, \quad \inf_{\theta \in J_n} |\lambda_n^{(3)}(\theta)| \geq Cn^{1/3}, \quad (10)$$

where C is a positive constant independent of n . By (10) and the estimates for the amplitude function (Proposition 14), we can prove Theorem 1 by using a lemma for estimating oscillatory integrals, given in Stein's book (see Stein [15, page 334] or Lemma 15 below). We can also prove the power $-1/3$ is optimal, by considering the case $s = \lambda'(\theta_0)$ (so, θ_0 is a stationary phase point), and applying the asymptotic expansion formula in the stationary phase method (see e.g. Stein [15, Page 334]).

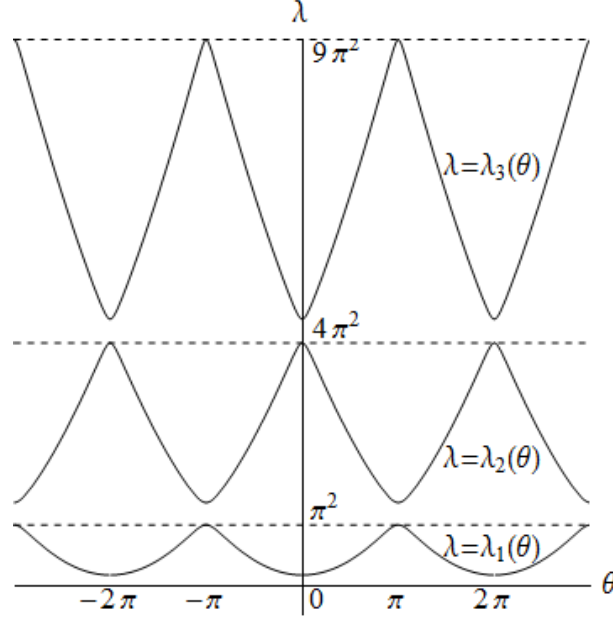


Figure 1: The graphs of the band functions $\lambda = \lambda_n(\theta)$ ($n = 1, 2, 3$) for $V > 0$. The range of $\lambda_n(\theta)$ is the n -th band I_n . We find two inflection points of $\lambda = \lambda_n(\theta)$ near $(n\pi, (n\pi)^2)$, for every n .

²All the graphs are written by using Mathematica 9.0.

The physical implication of the result is as follows. By definition, the parameter $s = ([x] - [y])/t$ represents the *propagation velocity* of a quantum particle. The wave packet with energy near $\lambda(\theta_0)$ has the maximal group speed in the n -th band, and the speed of the quantum diffusion is slowest in that band. Thus such state has a bit longer life-span (in the sense of L^∞ -norm) than the ordinary state has; the state is in some sense a *resonant state*, caused by the meeting of two stationary phase points θ_s as s tends to $s_0 = \lambda'(\theta_0)$. It is well-known that the existence of resonant states makes the decay of the solution with respect to t slower (see Jensen–Kato [6] or Mizutani [12]).

Since the estimate (8) is given bandwise, it is natural to ask we can obtain the dispersive type estimate for the whole Schrödinger time evolution operator e^{-itH} , like Cuccagna’s result (6). However, it turns out to be difficult in the present case, from the following reason. A reasonable strategy to prove such estimate is as follows. First, we divide the integral $K_{n,t}$ into two parts $\tilde{K}_{n,t}$ and the rest, where $\tilde{K}_{n,t}$ is given in (9) with J_n some open set including $\theta = 0, \pm\pi$. Next, we show the sum of $\tilde{K}_{n,t}$ converges and gives $O(t^{-1/3})$, and the sum of the rests also converges and gives $O(t^{-1/2})$. However, for fixed x and y , we find that our upper bound for $\tilde{K}_{n,t}(x, y)$ is not better than $O(n^{-1}t^{-1/2})$, and the sum of the upper bounds does not converge (see the last part of Section 4). One reason for this divergence is very strong singularity of our potential, the sum of δ -functions. Because of this singularity, the width of the band gap, say g_n (n is the band number), does not decay at all in the high energy limit $n \rightarrow \infty$.³ Then we cannot take the open set J_n so small,⁴ and the sum of the lengths $|J_n|$ diverges; if this sum converges, we can use a simple bound $|\tilde{K}_{n,t}| \leq C|J_n|$ to control the sum. Thus we do not succeed to obtain a bound for the sum of $\tilde{K}_{n,t}(x, y)$ at present.

On the other hand, for the Schrödinger operator $H = -d^2/dx^2 + V$ on \mathbf{R}^1 with real-valued periodic potential V , it is known that the decay rate of the width of the band gap g_n reflects the smoothness of the potential V . Hochstadt [5] says $g_n = o(n^{-(m-1)})$ if V is in C^m , and Trubowitz [16] says $g_n = O(e^{-cn})$ (c is some positive constant) if V is real analytic. So, if V is sufficiently smooth, it is expected that we can control the sum of $\tilde{K}_{n,t}$, and obtain the dispersive type estimate for the whole operator e^{-itH} (i.e. (8) without the projection P_n). We hope to argue this matter elsewhere in the near future.

The paper is organized as follows. In Section 2, we review the Floquet–Bloch theory for our operator H and give the explicit form of the integral kernel of e^{-itH} . In Section 3, we give more concrete analysis for the band functions, especially give some estimates for the derivatives. In Section 4, we prove Theorem 1, and give some comment for the summability with respect to n of the estimates (8).

2 Floquet–Bloch theory

In this section, we shall calculate the integral kernel of the operator e^{-itH} by using the Floquet–Bloch theory. Most results in this section are already written in another literature (e.g. Reed–Simon [14, XIII.16] and Albeverio et. al. [2, III.2.3]), but we shall give it here again for the completeness.

³ Proposition 10 implies $g_n \rightarrow 2|V|$ as $n \rightarrow \infty$.

⁴ We take $|J_n| = O(n^{-1/3})$ in the proof of Theorem 1.

First we shall calculate the generalized eigenfunctions for our model, i.e., the solutions to the equations

$$-\varphi''(x) = \lambda\varphi(x) \quad (x \in \mathbf{R} \setminus \mathbf{Z}), \quad (11)$$

$$\varphi(j+) = \varphi(j-) \quad (j \in \mathbf{Z}), \quad (12)$$

$$\varphi'(j+) - \varphi'(j-) = V\varphi(j) \quad (j \in \mathbf{Z}). \quad (13)$$

The condition (12) comes from the requirement $\varphi \in H_{\text{loc}}^1(\mathbf{R})$, and we use the abbreviation $\varphi(j) = \varphi(j\pm)$ in (13).

Proposition 2. *Let $\lambda \in \mathbf{C}$, $V \in \mathbf{R}$, and take $k \in \mathbf{C}$ so that $\lambda = k^2$. Then, the equations (11)-(13) have a solution $\varphi(x)$ of the following form.*

$$\varphi(x) = A_j \cos k(x - j) + B_j k^{-1} \sin k(x - j) \quad (j < x < j + 1), \quad (14)$$

where A_j and B_j are constants. When $k = 0$, we interpret $k^{-1} \sin k(x - j) = x - j$. The coefficients A_j and B_j satisfy the following recurrence relation.

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = T(k) \begin{pmatrix} A_{j-1} \\ B_{j-1} \end{pmatrix} \quad (j \in \mathbf{Z}), \quad (15)$$

$$T(k) = \begin{pmatrix} \cos k & k^{-1} \sin k \\ V \cos k - k \sin k & V k^{-1} \sin k + \cos k \end{pmatrix}.$$

The matrix $T(k)$ satisfies $\det T(k) = 1$ and the discriminant $D(k) = \text{tr } T(k)$ is

$$D(k) = 2 \cos k + V k^{-1} \sin k. \quad (16)$$

The proof is a simple calculation, so we shall omit it. Notice that $D(k) = D(\sqrt{\lambda})$ is an entire function with respect to λ , since $D(k)$ is an even function.

Next we shall calculate the *Bloch waves*, the solution to (11)-(13) with the quasi-periodic condition

$$\varphi(x + 1) = e^{i\theta} \varphi(x) \quad (x \in \mathbf{R} \setminus \mathbf{Z}) \quad (17)$$

for some $\theta \in \mathbf{R}$.

Proposition 3. *(i) For $\theta \in \mathbf{R}$, there exists a non-trivial solution φ to (11)-(13) satisfying the Bloch wave condition (17) if and only if*

$$D(k) = 2 \cos \theta. \quad (18)$$

(ii) When (18) holds, a solution $\varphi(x)$ to (11)-(13) and (17) is given by (14) with the coefficients

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} -k^{-1} \sin k \\ \cos k - e^{i\theta} \end{pmatrix}, \quad \begin{pmatrix} A_j \\ B_j \end{pmatrix} = e^{ij\theta} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \quad (j \in \mathbf{Z}). \quad (19)$$

Proof. (i) It is easy to see a non-trivial solution to (11)-(13) and (17) exists if and only if $T(k)$ has an eigenvalue $e^{i\theta}$, and the latter condition is equivalent to (18), since $\det T(k) = 1$ and $\text{tr } T(k) = D(k)$. (ii) When (18) holds, the vector $\begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$ given in (19) is an eigenvector of $T(k)$ with the eigenvalue $e^{i\theta}$. Thus the second equation in (19) follows from (15). \square

Proposition 3 and the Bloch theorem imply $\lambda \in \sigma(H)$ if and only if (18) holds for some $\theta \in \mathbf{R}$, that is,

$$-2 \leq D(\sqrt{\lambda}) \leq 2, \quad (20)$$

as already stated in (4). For $\lambda < 0$, we have

$$D(\sqrt{\lambda}) = 2 \cosh \sqrt{-\lambda} + V(\sqrt{-\lambda})^{-1} \sinh \sqrt{-\lambda}. \quad (21)$$

If $V > 0$, the right hand side of (21) is larger than 2 and (20) does not hold for $\lambda < 0$. Thus, there is no negative part in $\sigma(H)$. If $V < 0$, then some negative value λ belongs to $\sigma(H)$, and the corresponding k is pure imaginary. However, we concentrate on the high energy limit in the present paper, and the existence of the negative spectrum does not affect our argument. So we sometimes assume $V > 0$ in the sequel, in order to simplify the notation. In this case, the results for $V < 0$ will be stated in the remark.

By an elementary inspection of the graph of $y = D(k)$, we find the following properties.

Proposition 4. *Assume $V > 0$. Then,*

- (i) $D(0) = 2 + V$ and $D(n\pi) = 2 \cdot (-1)^n$ for $n = 1, 2, \dots$
- (ii) The equation $D(k) = 2 \cdot (-1)^n$ has a unique solution $k = k_n$ in the open interval $(n\pi, (n+1)\pi)$ for $n = 0, 1, 2, \dots$
- (iii) The equation $D'(k) = 0$ has a unique solution $k = l_n$ in the open interval $(n\pi, (n+1)\pi)$ for $n = 1, 2, \dots$, and $n\pi < l_n < k_n$.
- (iv) For convenience, we put $l_0 = 0$. Then, $D(k)$ is monotone decreasing on $[l_n, l_{n+1}]$ for even n , and monotone increasing on $[l_n, l_{n+1}]$ for odd n .

Remark. When $V < 0$, we denote the solution to $D(k) = 2 \cdot (-1)^n$ in $((n-1)\pi, n\pi)$ by k_n , and the solution to $D'(k) = 0$ in $((n-1)\pi, n\pi)$ by l_n , for $n = 2, 3, \dots$

When $V > 0$, the spectrum of H is given as

$$\sigma(H) = \bigcup_{n=1} I_n, \quad I_n = [k_{n-1}^2, (n\pi)^2], \quad (22)$$

by (20) and Proposition 4. The closed interval I_n is called the n -th band. By the expression (22), the band gap $((n\pi)^2, k_n^2)$ is non-empty for every $n = 1, 2, \dots$. Proposition 4 also implies the function $y = D(k)$ ($l_{n-1} \leq k \leq l_n$) has the unique inverse function $k = D^{-1}(y)$. Then the band function $\lambda_n(\theta)$ is defined by

$$\lambda_n(\theta) = (k(\theta))^2, \quad k(\theta) = D^{-1}(2 \cos \theta) \quad (k_{n-1} \leq k(\theta) \leq n\pi). \quad (23)$$

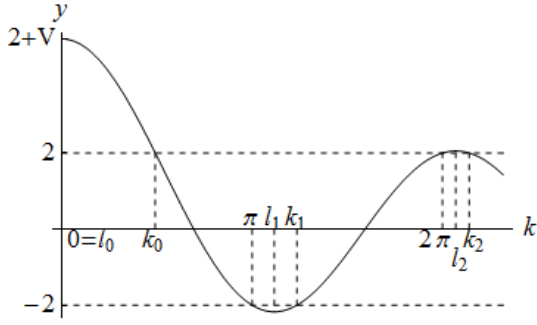


Figure 2: The graph of $y = D(k)$ when V is positive.

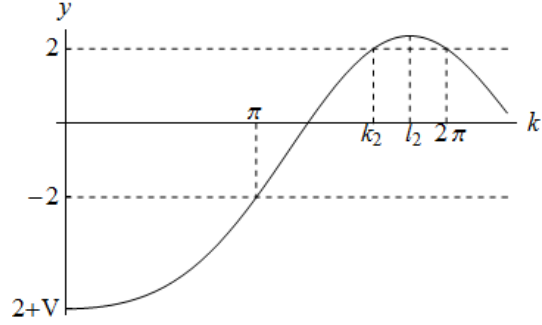


Figure 3: The graph of $y = D(k)$ when V is negative.

By definition, the band function $\lambda_n(\theta)$ is a real-analytic, periodic, and even function with respect to $\theta \in \mathbf{R}$. The n -th band I_n is the range of the band function λ_n .

Let P_n be the spectral projection for the self-adjoint operator H corresponding to the n -th band I_n . The spectral theorem implies

$$e^{-itH} = \text{s-}\lim_{N \rightarrow \infty} \sum_{n=1}^N P_n e^{-itH},$$

where s-lim means the strong limit in $L^2(\mathbf{R})$. Let $K_{n,t}(x, y)$ be the integral kernel of the operator $P_n e^{-itH}$, that is,

$$P_n e^{-itH} u(x) = \text{s-}\lim_{N \rightarrow \infty} \int_{-N}^N K_{n,t}(x, y) u(y) dy$$

for $u \in L^2(\mathbf{R})$. Let us calculate $K_{n,t}(x, y)$ more explicitly.

Proposition 5. *Assume $V > 0$. For $n = 1, 2, \dots$ and $\theta \in \mathbf{R}$, let $k = k(\theta)$ given by (23). Let $\varphi_{n,\theta}$ be the Bloch wave function defined by (14) and (19) with $k = k(\theta)$. Then, for any $x, y \in (0, 1)$ and $j, m \in \mathbf{Z}$, we have*

$$K_{n,t}(x + j, y + m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-itk^2 + i(j-m)\theta} \Phi_n(\theta, x, y) \cdot \frac{dk}{d\theta} d\theta, \quad (24)$$

$$\begin{aligned} \Phi_n(\theta, x, y) &= \frac{\sin k}{\sin \theta} \left(\cos kx + \frac{V}{2k} \sin kx \right) \left(\cos ky + \frac{V}{2k} \sin ky \right) \\ &\quad + i \sin k(x - y) + \frac{\sin \theta}{\sin k} \sin kx \sin ky, \end{aligned}$$

$$\frac{dk}{d\theta} = \frac{-2 \sin \theta}{D'(k)} = \frac{-2 \sin \theta}{-2 \sin k + V(k^{-1} \cos k - k^{-2} \sin k)}. \quad (25)$$

Remark. When $V < 0$, the same result holds for $n = 2, 3, \dots$, but the range of the function $k = k(\theta)$ is $[(n-1)\pi, k_n]$.

Before the proof, we prepare a lemma about the Wronskian of the Bloch waves. The Wronskian of two functions φ and ψ is defined as

$$W(\varphi, \psi) = \varphi\psi' - \varphi'\psi.$$

Lemma 6. (i) For any two solutions φ and ψ to (11)-(13), the Wronskian $W(\varphi, \psi)$ is a constant function on $\mathbf{R} \setminus \mathbf{Z}$.

(ii) Let $k = k(\theta)$ and $\varphi_{n,\theta}$ given in Proposition 5. Let $u_{n,\theta}$ be the normalized Bloch wave function defined by

$$u_{n,\theta} = \varphi_{n,\theta}/C_{n,\theta}, \quad C_{n,\theta} = \left(\int_0^1 |\varphi_{n,\theta}(x)|^2 dx \right)^{1/2}.$$

Then we have

$$\overline{u_{n,\theta}(x)} = u_{n,-\theta}(x), \quad (26)$$

$$k \frac{dk}{d\theta} = \frac{i}{2} W(u_{n,\theta}, u_{n,-\theta}), \quad (27)$$

Proof. (i) It is well-known that $W(\varphi, \psi)$ is constant on $(j, j+1)$ for every $j \in \mathbf{Z}$, since φ and ψ are solutions to (11). Moreover, (12) and (13) imply

$$\begin{aligned} W(\varphi, \psi)(j+) &= \det \begin{pmatrix} \varphi(j+) & \psi(j+) \\ \varphi'(j+) & \psi'(j+) \end{pmatrix} \\ &= \det \begin{pmatrix} 1 & 0 \\ V & 1 \end{pmatrix} \det \begin{pmatrix} \varphi(j-) & \psi(j-) \\ \varphi'(j-) & \psi'(j-) \end{pmatrix} = W(\varphi, \psi)(j-) \end{aligned}$$

for every $j \in \mathbf{Z}$. Thus $W(\varphi, \psi)$ is constant on $\mathbf{R} \setminus \mathbf{Z}$.

(ii) The first statement (26) follows immediately from the definition (14) and (19). We introduce an auxiliary function $v_{n,\theta}(x)$ by $u_{n,\theta}(x) = e^{ix\theta} v_{n,\theta}(x)$. Then we have

$$D(0)u_{n,\theta} = e^{ix\theta} D(\theta)v_{n,\theta}, \quad D(0) = \frac{1}{i} \frac{d}{dx}, \quad D(\theta) = \frac{1}{i} \frac{d}{dx} + \theta. \quad (28)$$

Since $\varphi = \varphi_{n,\theta}$ satisfies (11)-(13) and (17), it is easy to check

$$D(\theta)^2 v_{n,\theta}(x) = k^2 v_{n,\theta}(x) \quad (x \in \mathbf{R} \setminus \mathbf{Z}), \quad (29)$$

$$v_{n,\theta}(j+) = v_{n,\theta}(j-) \quad (j \in \mathbf{Z}), \quad (30)$$

$$v'_{n,\theta}(j+) - v'_{n,\theta}(j-) = V v_{n,\theta}(j) \quad (j \in \mathbf{Z}), \quad (31)$$

$$v_{n,\theta}(x+1) = v_{n,\theta}(x) \quad (x \in \mathbf{R} \setminus \mathbf{Z}). \quad (32)$$

In this proof, we denote (\cdot, \cdot) the inner product in $L^2((0, 1))$, that is, $(u, v) = \int_0^1 \overline{u(x)} v(x) dx$. Then we have from (29)

$$(v_{n,\theta}, v_{n,\theta}) = 1, \quad (33)$$

$$(v_{n,\theta}, D(\theta)^2 v_{n,\theta}) = k^2. \quad (34)$$

By differentiating both sides of (33) with respect to θ , we have

$$(\partial_\theta v_{n,\theta}, v_{n,\theta}) + (v_{n,\theta}, \partial_\theta v_{n,\theta}) = 0, \quad (35)$$

where $\partial_\theta = \partial/\partial\theta$. By differentiating both sides of (34) with respect to θ , we have

$$(\partial_\theta v_{n,\theta}, D(\theta)^2 v_{n,\theta}) + 2(v_{n,\theta}, D(\theta) v_{n,\theta}) + (v_{n,\theta}, D(\theta)^2 \partial_\theta v_{n,\theta}) = 2k \partial_\theta k. \quad (36)$$

By differentiating (30)-(32) with respect to θ , we see that the derivative $\partial_\theta v_{n,\theta}$ also satisfies the same relations (30)-(32). Then we have by integration by parts

$$(v_{n,\theta}, D(\theta)^2 \partial_\theta v_{n,\theta}) = (D(\theta)^2 v_{n,\theta}, \partial_\theta v_{n,\theta}). \quad (37)$$

By (29), (35) and (37), the first term and the third in the left hand side of (36) cancel with each other. Thus we have

$$\begin{aligned} k \partial_\theta k &= (v_{n,\theta}, D(\theta) v_{n,\theta}) \\ &= \frac{1}{2} ((v_{n,\theta}, D(\theta) v_{n,\theta}) + (D(\theta) v_{n,\theta}, v_{n,\theta})) \\ &= \frac{1}{2} ((u_{n,\theta}, D(0) u_{n,\theta}) + (D(0) u_{n,\theta}, u_{n,\theta})) \\ &= \frac{i}{2} \int_0^1 \left(-\overline{u_{n,\theta}(x)} u'_{n,\theta}(x) + \overline{u'_{n,\theta}(x)} u_{n,\theta}(x) \right) dx \\ &= \frac{i}{2} W(u_{n,\theta}, u_{n,-\theta}). \end{aligned}$$

Here we use (30)-(32) in the second equality, (28) in the third, and $\overline{u_{n,\theta}} = u_{n,-\theta}$ in the last. \square

Proof of Proposition 5. First, the Floquet-Bloch theory tells us

$$K_{n,t}(x, y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-it\lambda_n(\theta)} u_{n,\theta}(x) \overline{u_{n,\theta}(y)} d\theta \quad (38)$$

for any $x, y \in \mathbf{R}$. Actually, $u_{n,\theta}$ is the normalized eigenfunction of $H_\theta = H|_{\mathcal{H}_\theta}$, where \mathcal{H}_θ is the Hilbert space defined by

$$\mathcal{H}_\theta = \{u \in L^2_{\text{loc}}(\mathbf{R}) : u(x+1) = e^{i\theta} u(x)\}, \quad \|u\|_{\mathcal{H}_\theta}^2 = \int_0^1 |u(x)|^2 dx. \quad (39)$$

Since the whole operator H has the direct integral decomposition $H = \int_{[-\pi, \pi]}^\oplus H_\theta d\theta / (2\pi)$, the formula (38) follows from the eigenfunction expansion for H_θ (for the detail, see e.g. Reed-Simon [14]).

Let $x, y \in (0, 1)$ and $j, m \in \mathbf{Z}$. Since $\lambda_n(\theta) = k(\theta)^2$, $u_{n,\theta}(x+j) = e^{ij\theta} u_{n,\theta}(x)$, and $\overline{u_{n,\theta}(y)} = u_{n,-\theta}(y)$, we have from (38)

$$K_{n,t}(x+j, y+m) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-itk^2 + i(j-m)\theta} u_{n,\theta}(x) u_{n,-\theta}(y) \left(\frac{dk}{d\theta} \right)^{-1} \cdot \frac{dk}{d\theta} d\theta. \quad (40)$$

Moreover, we have by (27)

$$\left(\frac{dk}{d\theta}\right)^{-1} u_{n,\theta}(x)u_{n,-\theta}(y) = \frac{2k}{i} \frac{u_{n,\theta}(x)u_{n,-\theta}(y)}{W(u_{n,\theta}, u_{n,-\theta})} = \frac{2k}{i} \frac{\varphi_{n,\theta}(x)\varphi_{n,-\theta}(y)}{W(\varphi_{n,\theta}, \varphi_{n,-\theta})}. \quad (41)$$

The Wronskian $W(\varphi_{n,\theta}, \varphi_{n,-\theta})$ on the interval $(0, 1)$ is calculated as follows.

$$\begin{aligned} & W(\varphi_{n,\theta}, \varphi_{n,-\theta}) \\ &= \det \begin{pmatrix} A_0(\theta) \cos kx + B_0(\theta)k^{-1} \sin kx & A_0(-\theta) \cos kx + B_0(-\theta)k^{-1} \sin kx \\ -kA_0(\theta) \sin kx + B_0(\theta) \cos kx & -kA_0(-\theta) \sin kx + B_0(-\theta) \cos kx \end{pmatrix} \\ &= \det \begin{pmatrix} \cos kx & k^{-1} \sin kx \\ -k \sin kx & \cos kx \end{pmatrix} \det \begin{pmatrix} A_0(\theta) & A_0(-\theta) \\ B_0(\theta) & B_0(-\theta) \end{pmatrix} \\ &= A_0(\theta)B_0(-\theta) - A_0(-\theta)B_0(\theta) \\ &= -k^{-1} \sin k(\cos k - e^{-i\theta}) + k^{-1} \sin k(\cos k - e^{i\theta}) \\ &= -2ik^{-1} \sin k \sin \theta. \end{aligned} \quad (42)$$

By (16) and (18), we have

$$e^{i\theta} = \cos k + \frac{V}{2}k^{-1} \sin k + i \sin \theta.$$

This equality and (19) implies for $0 < x < 1$

$$\begin{aligned} \varphi_{n,\theta}(x) &= A_0(\theta) \cos kx + B_0(\theta) \sin kx \\ &= -k^{-1} \sin k \left(\cos kx + \frac{V}{2k} \sin kx \right) - ik^{-1} \sin \theta \sin kx. \end{aligned} \quad (43)$$

Substituting (42) and (43) into (41), we have

$$\begin{aligned} & \left(\frac{dk}{d\theta}\right)^{-1} u_{n,\theta}(x)u_{n,-\theta}(y) \\ &= \frac{k^2}{\sin k \sin \theta} \varphi_{n,\theta}(x)\varphi_{n,-\theta}(y) \\ &= \frac{1}{\sin k \sin \theta} \left(\sin k \left(\cos kx + \frac{V}{2k} \sin kx \right) + i \sin \theta \sin kx \right) \\ & \quad \cdot \left(\sin k \left(\cos ky + \frac{V}{2k} \sin ky \right) - i \sin \theta \sin ky \right) \\ &= \Phi_n(\theta, x, y). \end{aligned}$$

Substituting this equality into (40), we have (24). The derivative (25) is obtained by differentiating $2 \cos \theta = D(k) = 2 \cos k + Vk^{-1} \sin k$. \square

Remark. Note that $dk/d\theta$ is positive for $0 < \theta < \pi$ for odd n , and negative for even n . Substituting (41) into (40) and making the change of variable $\lambda = (k(\theta))^2$, we have

for $V > 0$

$$\begin{aligned} K_{n,t}(x, y) &= \frac{1}{i\pi} \int_{-\pi}^{\pi} e^{-itk^2} \frac{\varphi_{n,\theta}(x) \varphi_{n,-\theta}(y)}{W(\varphi_{n,\theta}, \varphi_{n,-\theta})} k \cdot \frac{dk}{d\theta} d\theta \\ &= \frac{(-1)^{n-1}}{\pi} \int_{k_{n-1}^2}^{(n\pi)^2} e^{-it\lambda} \operatorname{Im} \left[\frac{\varphi_{n,\theta}(x) \varphi_{n,-\theta}(y)}{W(\varphi_{n,\theta}, \varphi_{n,-\theta})} \right] d\lambda. \end{aligned} \quad (44)$$

The formula (44) can be deduced in another way. According to the Stone formula ([13, Theorem VII.13]), the spectral measure E_H for the operator H is represented as

$$\frac{dE_H}{d\lambda} = \frac{1}{\pi} \operatorname{Im} R_H(\lambda + i0), \quad (45)$$

where $R_H(\lambda + 0) = \lim_{\epsilon \rightarrow +0} R(\lambda + i\epsilon)$ is the boundary value of the resolvent $R(\lambda) = (H - \lambda)^{-1}$. The integral kernel of the resolvent operator $R(\lambda)$ for $\lambda \in \rho(H)$ (the resolvent set of H) is given as

$$R(\lambda)(x, y) = -\frac{\varphi_+^\lambda(x \vee y) \varphi_-^\lambda(x \wedge y)}{W(\varphi_+^\lambda, \varphi_-^\lambda)}, \quad (46)$$

where $x \vee y = \max(x, y)$, $x \wedge y = \min(x, y)$, and φ_\pm^λ is the solution to (11)-(13) decaying exponentially as $x \rightarrow \pm\infty$. The two functions φ_\pm^λ are given by (14) and (19) with $e^{i\theta}$ replaced by the solutions to

$$z^2 - D(\sqrt{\lambda})z + 1 = 0,$$

so that $|z|^{\pm 1} < 1$. By choosing the solution z appropriately, (45) and (46) give the formula (44).

3 Analysis of band functions

In this section, we analyze the band function $\lambda_n(\theta)$, which is explicitly given by

$$\lambda_n(\theta) = (k(\theta))^2, \quad k(\theta) = D^{-1}(2 \cos \theta), \quad (47)$$

especially its asymptotics as $n \rightarrow \infty$. Here $k = D^{-1}(y)$ is the inverse function of

$$y = D(k) = 2 \cos k + V \frac{\sin k}{k} : [l_{n-1}, l_n] \rightarrow [y_{n-1}, y_n],$$

l_n is given in Proposition 4 and its remark, and we put $y_n = D(l_n)$. By the formula (47), we can draw the graphs of $\lambda_n(\theta)$,⁵ which are illustrated in Figure 1 in the introduction. From Figure 1, we notice that $\lambda = \lambda_n(\theta)$ is similar to the parabola $\lambda = \theta^2$ on the interval $[(n-1)\pi, n\pi]$, except near the edge points. From this reason, we mainly consider the function $\lambda_n(\theta)$ on the interval $[(n-1)\pi, n\pi]$, thereby we can simplify some formulas given below. Figure 1 also suggests us it is better to analyze $\lambda_n(\theta)$ when its value is near the band edge, and near the band center, separately.

⁵ The inverse correspondence $\theta = \arccos(D(k)/2)$ is useful for the numerical calculation.

3.1 Explicit formulas for derivatives

Our goal is to give an asymptotic bound for the oscillatory integral (24), by using Lemma 15 in Section 4. Then we need lower bounds for the derivatives of $\lambda_n(\theta)$ up to the third order, which are calculated explicitly as follows.

$$k'(\theta) = -D'(k)^{-1} \cdot 2 \sin \theta, \quad (48)$$

$$\begin{aligned} k''(\theta) &= (D^{-1})''(2 \cos \theta) \cdot (2 \sin \theta)^2 - (D^{-1})'(2 \cos \theta) \cdot 2 \cos \theta \\ &= -D'(k)^{-3} D''(k) (4 - D(k)^2) - D'(k)^{-1} D(k), \end{aligned} \quad (49)$$

$$\begin{aligned} k^{(3)}(\theta) &= -(D^{-1})^{(3)}(2 \cos \theta) \cdot (2 \sin \theta)^3 + 3 \cdot (D^{-1})''(2 \cos \theta) \cdot 2 \sin \theta \cdot 2 \cos \theta \\ &\quad + (D^{-1})'(2 \cos \theta) \cdot 2 \sin \theta, \\ &= \left((-3D'(k)^{-5} D''(k)^2 + D'(k)^{-4} D^{(3)}(k)) (4 - D(k)^2) \right. \\ &\quad \left. - 3D'(k)^{-3} D(k) D''(k) + D'(k)^{-1} \right) \cdot 2 \sin \theta, \end{aligned} \quad (50)$$

$$\lambda'_n(\theta) = 2k(\theta)k'(\theta), \quad (51)$$

$$\lambda''_n(\theta) = 2k'(\theta)^2 + 2k(\theta)k''(\theta), \quad (52)$$

$$\lambda_n^{(3)}(\theta) = 6k'(\theta)k''(\theta) + 2k(\theta)k^{(3)}(\theta), \quad (53)$$

where we used the formulas

$$2 \cos \theta = D(k), \quad (2 \sin \theta)^2 = 4 - D(k)^2, \quad (54)$$

$$(D^{-1})'(D(k)) = D'(k)^{-1}, \quad (D^{-1})''(D(k)) = -D'(k)^{-3} D''(k), \quad (55)$$

$$(D^{-1})^{(3)}(D(k)) = 3D'(k)^{-5} D''(k)^2 - D'(k)^{-4} D^{(3)}(k).$$

The derivatives of $D(k)$ are given as follows.

$$D(k) = 2 \cos k + V k^{-1} \sin k, \quad (56)$$

$$D'(k) = -2 \sin k + V(k^{-1} \cos k - k^{-2} \sin k), \quad (57)$$

$$D''(k) = -2 \cos k + V(-k^{-1} \sin k - 2k^{-2} \cos k + 2k^{-3} \sin k), \quad (58)$$

$$D^{(3)}(k) = 2 \sin k + V(-k^{-1} \cos k + 3k^{-2} \sin k + 6k^{-3} \cos k - 6k^{-4} \sin k), \quad (59)$$

$$\begin{aligned} D^{(4)}(k) &= 2 \cos k + V(k^{-1} \sin k + 4k^{-2} \cos k - 12k^{-3} \sin k - 24k^{-4} \cos k \\ &\quad + 24k^{-5} \sin k), \end{aligned} \quad (60)$$

$$\begin{aligned} D^{(5)}(k) &= -2 \sin k + V(k^{-1} \cos k - 5k^{-2} \sin k - 20k^{-3} \cos k + 60k^{-4} \sin k \\ &\quad + 120k^{-5} \cos k - 120k^{-6} \sin k), \end{aligned} \quad (61)$$

$$\begin{aligned} D^{(6)}(k) &= -2 \cos k + V(-k^{-1} \sin k - 6k^{-2} \cos k + 30k^{-3} \sin k + 120k^{-4} \cos k \\ &\quad - 360k^{-5} \sin k - 720k^{-6} \cos k + 720k^{-7} \sin k). \end{aligned} \quad (62)$$

By the formulas (48)-(53), we can write $\lambda_n^{(j)}(\theta)$ ($j = 1, 2, 3$) as functions of k , which is useful for numerical calculation. The graphs of $\lambda'_n(\theta)$ and $\lambda''_n(\theta)$ on the interval $(n-1)\pi \leq \theta \leq n\pi$ ($n = 1, 2, 3, 4, 5$) are illustrated in Figure 4 and Figure 5, respectively. From Figure 5, we see that the solution θ_0 to $\lambda''_n(\theta) = 0$ exists nearby $\theta = n\pi$. Later we give the asymptotics of θ_0 as $n \rightarrow \infty$ in Proposition 11.

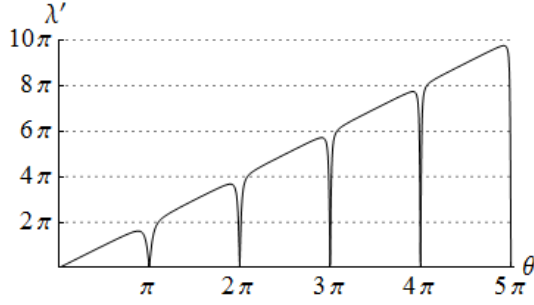


Figure 4: The graphs of $\lambda'_n(\theta)$ on $[(n-1)\pi, n\pi]$ ($n = 1, 2, 3, 4, 5$) for $V > 0$.

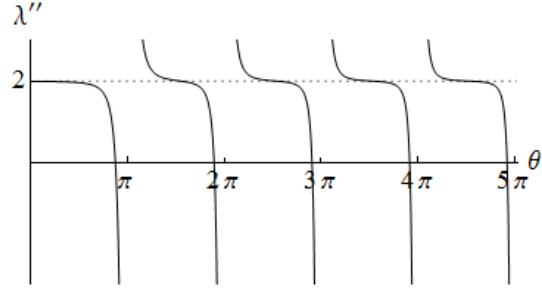


Figure 5: The graphs of $\lambda''_n(\theta)$ on $[(n-1)\pi, n\pi]$ ($n = 1, 2, 3, 4, 5$) for $V > 0$.

Though the formulas (48)-(53) are explicit, it is still not easy to obtain the precise lower bound for the derivatives of $\lambda_n(\theta)$, especially when $\lambda_n(\theta)$ is near the band edge. For this reason, we employ the *Puiseux expansion* of the inverse function $D^{-1}(y)$, which makes our analysis clear. This kind of expansion is studied in the classical work by Kohn [7].

3.2 Asymptotics of k_n and l_n

First let us analyze the asymptotics of k_n and l_n given in Proposition 4. A related result is written in Albeverio et. al. [2, Theorem 2.3.3].

Proposition 7. *Let k_n and l_n as in Proposition 4 and its remark. Then,*

$$k_n = n\pi + V(n\pi)^{-1} - \left(V^2 + \frac{V^3}{12}\right)(n\pi)^{-3} + O(n^{-5}) \quad (n \rightarrow \infty), \quad (63)$$

$$l_n = n\pi + \frac{V}{2}(n\pi)^{-1} - \left(\frac{V^2}{2} + \frac{V^3}{24}\right)(n\pi)^{-3} + O(n^{-5}) \quad (n \rightarrow \infty). \quad (64)$$

Proof. We assume $V > 0$ for simplicity (in the case $V < 0$, we only need to change the sign of h given below). First we prove (63). The number k_n is the solution to

$$D(k) = 2 \cos k + V \frac{\sin k}{k} = 2(-1)^n \quad (n\pi < k < (n+1)\pi). \quad (65)$$

Put $k = n\pi + h$. Then (65) is equivalent to

$$h = f(h), \quad f(h) = \arcsin \left(\frac{1 + \cos h}{2} \frac{V}{n\pi + h} \right). \quad (66)$$

Then, for sufficiently large n , it is easy to see that the solution to (66) is the limit of the sequence $\{h_j\}_{j=0}$ given by⁶

$$h_0 = 0, \quad h_j = f(h_{j-1}) \quad (j = 1, 2, \dots). \quad (67)$$

⁶For the rigorous proof, we apply the contraction mapping theorem in the following form: ‘Let $I = [a, b]$, $0 \in I$, $f \in C^1(I)$ and assume $f(I) \subset I$ and $\|f'\|_{L^\infty(I)} < 1$. Then f has the unique fixed point in I which is the limit of the sequence (67)’. If we take f as in (66) and $I = [0, 2V/(n\pi)]$, we can apply the contraction mapping theorem for sufficiently large n .

By a simple calculation, we have

$$f(h) = \frac{V}{n\pi} - \frac{V}{(n\pi)^2}h - \frac{V}{4n\pi}h^2 + \frac{1}{6} \frac{V^3}{(n\pi)^3} + O(n^{-5}) \quad \text{for } h = O(n^{-1}). \quad (68)$$

Then twice substitution of (68) into (67) gives the formula (63) (three times substitution gives the same formula).

Next we prove (64). Put $k = n\pi + h$. Then the defining equation of l_n

$$D'(k) = -2 \sin k + V(k^{-1} \cos k - k^{-2} \sin k) = 0$$

is equivalent to

$$h = g(h), \quad g(h) = \arctan \left(\frac{Vk}{2k^2 + V} \right), \quad k = n\pi + h.$$

Then we can obtain the formula (64) by using the following expansion recursively.

$$g(h) = \frac{V}{2n\pi} - \frac{V^2}{4(n\pi)^3} - \frac{V}{2(n\pi)^2}h - \frac{1}{24} \frac{V^3}{(n\pi)^3} + O(n^{-5}) \quad \text{for } h = O(n^{-1}).$$

□

3.3 Analysis on $\lambda_n(\theta)$ near the band edge

In order to calculate the Puiseux expansion of $k = D^{-1}(y)$, first we calculate the Taylor expansion of $y = D(k)$.

Proposition 8. *The Taylor expansion of $y = D(k)$ near $k = l_n$ is given as follows.*

$$y = D(k) = y_n + \sum_{m=2}^{\infty} d_m (k - l_n)^m, \quad y_n = D(l_n), \quad d_m = \frac{D^{(m)}(l_n)}{m!}, \quad (69)$$

$$y_n = (-1)^n \left[2 + \frac{V^2}{4} (n\pi)^{-2} + O(n^{-4}) \right], \quad (70)$$

$$d_2 = (-1)^n \left[-1 - \left(V + \frac{V^2}{8} \right) (n\pi)^{-2} + O(n^{-4}) \right], \quad (71)$$

$$d_3 = (-1)^n \left[\left(V + \frac{V^2}{6} \right) (n\pi)^{-3} + O(n^{-5}) \right], \quad (72)$$

$$d_4 = (-1)^n \left[\frac{1}{12} + \left(\frac{V}{6} + \frac{V^2}{96} \right) (n\pi)^{-2} + O(n^{-4}) \right], \quad (73)$$

$$d_5 = (-1)^n \left[- \left(\frac{V}{6} + \frac{V^2}{60} \right) (n\pi)^{-3} + O(n^{-5}) \right], \quad (74)$$

$$d_6 = (-1)^n \left[-\frac{1}{360} - \left(\frac{V}{120} + \frac{V^2}{2880} \right) (n\pi)^{-2} + O(n^{-4}) \right]. \quad (75)$$

Proof. Notice that $d_1 = D'(l_n) = 0$ by definition. The results (70)-(74) can be obtained by substituting the following formulas into (56)-(62). From (64), we have

$$\begin{aligned} (-1)^n \cos l_n &= 1 - \frac{V^2}{8}(n\pi)^{-2} + O(n^{-4}), \\ (-1)^n \sin l_n &= \frac{V}{2}(n\pi)^{-1} - \left(\frac{V^2}{2} + \frac{V^3}{16} \right) (n\pi)^{-3} + O(n^{-5}), \\ l_n^{-1} &= (n\pi)^{-1} - \frac{V}{2}(n\pi)^{-3} + O(n^{-5}), \\ l_n^{-j} &= (n\pi)^{-j} + O(n^{-(j+2)}) \quad (j \geq 2). \end{aligned}$$

□

Next we shall calculate the Puiseux expansion of $D^{-1}(y)$ near $y = y_n$. Since $k = k_n$ is the zero of order 2 of $D(k)$, $D^{-1}(y)$ is a double-valued function with respect to the complex variable y .

Proposition 9. *The Puiseux expansion of $k = D^{-1}(y)$ near $y = y_n$ is written as follows.*

$$k = l_n + \sum_{p=1}^{\infty} e_p h^{p/2}, \quad h = (-1)^n (y_n - y), \quad (76)$$

$$e_1 = 1 - \left(\frac{V}{2} + \frac{V^2}{16} \right) (n\pi)^{-2} + O(n^{-4}), \quad (77)$$

$$e_2 = \left(\frac{V}{2} + \frac{V^2}{12} \right) (n\pi)^{-3} + O(n^{-5}), \quad (78)$$

$$e_3 = \frac{1}{24} - \left(\frac{V}{48} + \frac{V^2}{128} \right) (n\pi)^{-2} + O(n^{-4}), \quad (79)$$

$$e_4 = \left(\frac{V}{24} + \frac{V^2}{80} \right) (n\pi)^{-3} + O(n^{-5}), \quad (80)$$

$$e_5 = \frac{3}{640} - \left(\frac{3V}{1280} + \frac{3V^2}{2048} \right) (n\pi)^{-2} + O(n^{-4}). \quad (81)$$

Proof. Put $h = (-1)^n (y_n - y)$ and $c_m = (-1)^{n+1} d_m$, where d_m are the coefficients in (69). Then the Taylor expansion (69) is rewritten as

$$h = \sum_{m=2}^{\infty} c_m (k - l_n)^m. \quad (82)$$

Substituting the Puiseux expansion (76) into (82), and comparing the coefficient of each

power $h^{p/2}$, we have

$$\begin{aligned}
c_2 e_1^2 &= 1, \\
2c_2 e_1 e_2 + c_3 e_1^3 &= 0, \\
c_2(2e_1 e_3 + e_2^2) + 3c_3 e_1^2 e_2 + c_4 e_1^4 &= 0, \\
c_2(2e_1 e_4 + 2e_2 e_3) + c_3(3e_1^2 e_3 + 3e_1 e_2^2) + 4c_4 e_1^3 e_2 + c_5 e_1^5 &= 0, \\
c_2(2e_1 e_5 + 2e_2 e_4 + e_3^2) + c_3(6e_1 e_2 e_3 + 3e_1^2 e_4 + e_2^3) + c_4(6e_1^2 e_2^2 + 4e_1^3 e_3) \\
&\quad + 5c_5 e_1^4 e_2 + c_6 e_1^6 = 0.
\end{aligned}$$

Since the expansions of $c_m = (-1)^{n+1} d_m$ are obtained from (71)-(75), we can calculate the coefficients (77)-(81) by solving the above equations. \square

Remark. 1. The branch points of $k = D^{-1}(y)$ are $y = y_n$, and y_n is nearby $2 \cdot (-1)^n$ by (70). Thus the radius of convergence of the Puiseux expansion (76) is about 4, for sufficiently large n . This fact justifies the calculus in the sequel.

2. In the case $V = 0$, the expansion (76) coincides with the Puiseux expansion

$$\arccos \frac{y}{2} = n\pi + (2 \mp y)^{1/2} + \frac{1}{24}(2 \mp y)^{3/2} + \frac{3}{640}(2 \mp y)^{5/2} + \cdots \quad (\text{near } y = \pm 2),$$

where n is any integer satisfying $(-1)^n = \pm 1$.

Substituting $y = 2 \cos \theta$ into (76), we obtain the function $k = k(\theta) = D^{-1}(2 \cos \theta)$. Since the Puiseux expansion (76) has two branches, we obtain two functions

$$k_{\pm}(\theta) = l_n \pm e_1 h^{1/2} + e_2 h \pm e_3 h^{3/2} + e_4 h^2 \pm e_5 h^{5/2} + \cdots, \quad (83)$$

$$h = (-1)^n (y_n - 2 \cos \theta). \quad (84)$$

Notice that h is positive for real θ , so $h^{p/2}$ in (83) is uniquely defined as a positive function. For notational simplicity, we put

$$z_n = (-1)^n y_n, \quad \theta = n\pi + \tau. \quad (85)$$

Then we have the following formulas, useful for the calculation below.

$$z_n = 2 + \frac{V^2}{4}(n\pi)^{-2} + O(n^{-4}), \quad (86)$$

$$h = z_n - 2 \cos \tau = \tau^2 + O(\tau^4) + \frac{V^2}{4}(n\pi)^{-2} + O(n^{-4}), \quad (87)$$

$$\frac{dh}{d\tau} = 2 \sin \tau, \quad (88)$$

$$(2 \sin \tau)^2 = 4 - (2 \cos \tau)^2 = (4 - z_n^2) + 2z_n h - h^2, \quad (89)$$

$$4 - z_n^2 = -V^2(n\pi)^{-2} + O(n^{-4}). \quad (90)$$

Then we obtain expansions of the band functions and their derivatives near the band edge, as follows.

Proposition 10. *Let k_{\pm} , h and τ as in (83)-(85), and put $\lambda_{\pm}(\theta) = k_{\pm}(\theta)^2$. Then the following expansions hold near $\theta = n\pi$ (or $\tau = 0$).*

(i)

$$\lambda_{\pm} = l_n^2 \pm \lambda_{0,1}h^{1/2} + \lambda_{0,2}h \pm \lambda_{0,3}h^{3/2} + \lambda_{0,4}h^2 \pm \lambda_{0,5}h^{5/2} + O(h^3),$$

$$l_n^2 = (n\pi)^2 + V - \left(\frac{3V^2}{4} + \frac{V^3}{12} \right) (n\pi)^{-2} + O(n^{-4}),$$

$$\lambda_{0,1} = 2n\pi - \frac{V^2}{8}(n\pi)^{-1} + O(n^{-3}),$$

$$\lambda_{0,2} = 1 + \frac{V^2}{24}(n\pi)^{-2} + O(n^{-4}),$$

$$\lambda_{0,3} = \frac{1}{12}n\pi - \frac{V^2}{64}(n\pi)^{-1} + O(n^{-3}),$$

$$\lambda_{0,4} = \frac{1}{12} + \frac{V^2}{240}(n\pi)^{-2} + O(n^{-4}),$$

$$\lambda_{0,5} = \frac{3}{320}n\pi - \frac{3V^2}{1024}(n\pi)^{-1} + O(n^{-3}).$$

(ii)

$$\frac{d\lambda_{\pm}}{d\theta} = 2 \sin \tau \cdot \left(\pm \frac{1}{2}\lambda_{0,1}h^{-1/2} + \lambda_{0,2} \pm \frac{3}{2}\lambda_{0,3}h^{1/2} + 2\lambda_{0,4}h \pm \frac{5}{2}\lambda_{0,5}h^{3/2} + O(h^2) \right). \quad (91)$$

(iii)

$$\frac{d^2\lambda_{\pm}}{d\theta^2} = \pm\lambda_{2,-3}h^{-3/2} \pm \lambda_{2,-1}h^{-1/2} + \lambda_{2,0} \pm \lambda_{2,1}h^{1/2} + O(h), \quad (92)$$

$$\lambda_{2,-3} = \frac{V^2}{2}(n\pi)^{-1} + O(n^{-3}), \quad (93)$$

$$\lambda_{2,-1} = -\frac{V^2}{16}(n\pi)^{-1} + O(n^{-3}), \quad (94)$$

$$\lambda_{2,0} = 2 + \frac{V^2}{6}(n\pi)^{-2} + O(n^{-4}), \quad (95)$$

$$\lambda_{2,1} = -\frac{9V^2}{256}(n\pi)^{-1} + O(n^{-3}). \quad (96)$$

(iv)

$$\frac{d^3\lambda_{\pm}}{d\theta^3} = 2 \sin \tau \cdot \left(\mp \frac{3}{2}\lambda_{2,-3}h^{-5/2} \mp \frac{1}{2}\lambda_{2,-1}h^{-3/2} \pm \frac{1}{2}\lambda_{2,1}h^{-1/2} + O(1) \right). \quad (97)$$

Proof. The proof can be done simply by substituting the expansion (83), (64) and (77)-(81) into $\lambda_{\pm} = k_{\pm}^2$ and taking the derivative with respect to θ (or τ) repeatedly. The formulas (86)-(90) help the calculation. \square

By construction, we have

$$\lambda_+(\theta) = \lambda_{n+1}(\theta), \quad \lambda_-(\theta) = \lambda_n(\theta), \quad \theta = n\pi + \tau \quad (98)$$

for small τ . Using (98) and the expansion (92), we can find the asymptotics of the solution to $\lambda_n''(\theta) = 0$.

Proposition 11. *The equation*

$$\frac{d^2\lambda_n}{d\theta^2} = 0, \quad (n-1)\pi \leq \theta \leq n\pi$$

has a unique solution $\theta = \theta_0$ for sufficiently large n . The asymptotics of θ_0 is given as

$$\theta_0 = n\pi - \left(\frac{V^2}{4n\pi}\right)^{1/3} + O(n^{-1}) \quad \text{as } n \rightarrow \infty. \quad (99)$$

Before the proof, we give a numerical result by using the explicit formulas (48)-(53), in Figure 6. The result shows the formula (99) gives a good approximation.

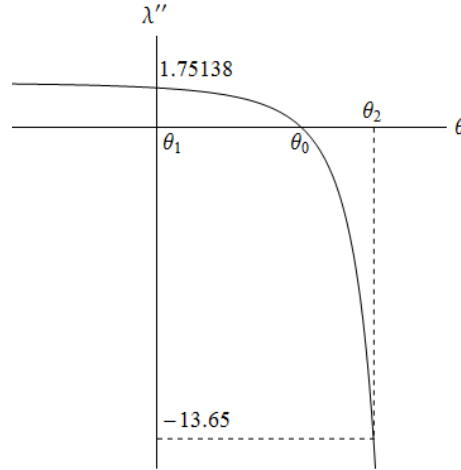


Figure 6: The graph of $\lambda_n''(\theta)$ near $\theta_0 = n\pi - \delta_n^{1/3}$, $\delta_n = V^2/(4n\pi)$. Here we take $V = 1$, $n = 1000$, $\theta_1 = n\pi - 2\delta_n^{1/3}$, and $\theta_2 = n\pi - \delta_n^{1/3}/2$.

Proof. Put $\delta_n = V^2/(4n\pi)$. We divide the interval $[(n-1)\pi, n\pi]$ into three intervals

$$\begin{aligned} I_1 &= [(n-1)\pi, (n-1)\pi + \delta_n^{1/4}], & I_2 &= [(n-1)\pi + \delta_n^{1/4}, n\pi - \delta_n^{1/4}], \\ I_3 &= [n\pi - \delta_n^{1/4}, n\pi]. \end{aligned}$$

For $\theta \in I_1$, we apply the first equality of (98) with n replaced by $n-1$, so $\lambda_n = \lambda_+$ and $\theta = (n-1)\pi + \tau$. Then the expansion (92) for $d^2\lambda_+/d\theta^2$ implies $\lambda_n''(\theta) > 0$ for $\theta \in I_1$,

for sufficiently large n . Moreover, the formula (107) given later in Proposition 13 shows $\lambda_n''(\theta) > 0$ for $\theta \in I_2$, for sufficiently large n .

For $\theta \in I_3$, we apply the second equality of (98), so $\lambda_n = \lambda_-$ and $\theta = n\pi + \tau$. Then $-\delta_n^{1/4} < \tau < 0$, and (97) for λ_- implies $\lambda_n^{(3)}(\theta) < 0$ for $\theta \in I_3 \setminus \{n\pi\}$, for sufficiently large n . Thus $\lambda_n''(\theta)$ is monotone decreasing on this interval, and (92) for $d^2\lambda_-/d\theta^2$ implies $\lambda_n''(n\pi - \delta_n^{1/4}) > 0$ and $\lambda_n''(n\pi) < 0$ for sufficiently large n .⁷ Thus there exists a unique $\theta_0 \in [(n-1)\pi, n\pi]$ with $\lambda_n''(\theta_0) = 0$ for sufficiently large n , and $\theta_0 \in I_3$.

Let us find more detailed asymptotics of θ_0 . By (92) for $d^2\lambda_-/d\theta^2$,

$$\begin{aligned} \frac{d^2\lambda_n}{d\theta^2} = 0 &\Leftrightarrow -\lambda_{2,-3}h^{-3/2} - \lambda_{2,-1}h^{-1/2} + \lambda_{2,0} - \lambda_{2,1}h^{1/2} + O(h) = 0 \\ &\Leftrightarrow h = f(h), \quad f(h) = \left(\frac{\lambda_{2,-3} + \lambda_{2,-1}h + \lambda_{2,1}h^2 + O(h^{5/2})}{\lambda_{2,0}} \right)^{2/3}. \end{aligned} \quad (100)$$

If $\theta \in I_3$, then $\tau = O(n^{-1/4})$ and $h = O(n^{-1/2})$ by (87). So, if h is the solution to (100), the expansions of the coefficients (93)-(96) imply $h = O(n^{-2/3})$, and again by (100)

$$\begin{aligned} h = f(h) &= (\delta_n + O(n^{-5/3}))^{2/3} \\ &= \delta_n^{2/3} (1 + O(n^{-2/3})). \end{aligned} \quad (101)$$

Thus (101) and (87) imply

$$\tau = -\delta_n^{1/3} + O(n^{-1}).$$

Since $\theta = n\pi + \tau$, we have the conclusion. \square

3.4 Analysis on $\lambda_n(\theta)$ near the band center

Let us prove $\lambda_n(\theta)$ is similar to the parabola $\lambda = \theta^2$ near the band center, that is, for θ in the interval

$$\left[(n-1)\pi + \left(\frac{V^2}{4n\pi} \right)^{1/4}, n\pi - \left(\frac{V^2}{4n\pi} \right)^{1/4} \right]. \quad (102)$$

Notice that the asymptotics (99) implies θ_0 is not in the interval (102) for large n .

Lemma 12. *Let $k(\theta) = D^{-1}(2 \cos \theta)$ given in (47), and θ in the interval (102). Then, we have the following expansion.*

$$\begin{aligned} k &= \theta - VD'(\theta)^{-1} \frac{\sin \theta}{\theta} - \frac{V^2}{2} D'(\theta)^{-3} D''(\theta) \left(\frac{\sin \theta}{\theta} \right)^2 + R_3, \\ R_3 &= -V^3 \left(\frac{\sin \theta}{\theta} \right)^3 \int_0^1 \frac{(1-z)^2}{2} (D^{-1})^{(3)} \left(D(\theta) - zV \frac{\sin \theta}{\theta} \right) dz. \end{aligned} \quad (103)$$

Remark. The explicit forms of the derivatives are given in (56)-(62).

⁷When $V > 0$, the latter fact can also be proved by the explicit value $\lambda_n''(n\pi) = -4(n\pi)^2/V$; see ((138) below).

Proof. The Taylor expansion of $k = D^{-1}(y)$ around $y = D(\theta)$ is

$$\begin{aligned} k &= D^{-1}(D(\theta)) + (D^{-1})'(D(\theta)) \cdot (y - D(\theta)) \\ &\quad + \frac{(D^{-1})''(D(\theta))}{2} \cdot (y - D(\theta))^2 + R_3(y), \end{aligned} \quad (104)$$

$$R_3(y) = (y - D(\theta))^3 \cdot \int_0^1 \frac{(1-z)^2}{2} (D^{-1})^{(3)}(D(\theta) + z(y - D(\theta))) dz. \quad (105)$$

Substituting the equality

$$y = 2 \cos \theta = D(\theta) - V \frac{\sin \theta}{\theta}$$

into (104) and (105), we obtain the conclusion since

$$\begin{aligned} D^{-1}(D(\theta)) &= \theta, \\ (D^{-1})'(D(\theta)) &= D'(\theta)^{-1}, \\ (D^{-1})''(D(\theta)) &= -D'(\theta)^{-3} D''(\theta), \end{aligned}$$

where we used (55). □

Proposition 13. *Let n be a sufficiently large integer. Then, for θ in the interval (102), we have the expansion of $k = D^{-1}(2 \cos \theta)$ given in (47) as follows.*

$$\begin{aligned} k &= \theta + \frac{V}{2\theta} + \frac{V^2}{8\theta^2} \cot \theta + O(n^{-5/2}), \\ \frac{dk}{d\theta} &= 1 - \frac{V}{2\theta^2} - \frac{V^2}{8\theta^2 \sin^2 \theta} + O(n^{-9/4}), \\ \frac{d^2 k}{d\theta^2} &= \frac{V^2 \cos \theta}{4\theta^2 \sin^3 \theta} + O(n^{-2}). \end{aligned} \quad (106)$$

Moreover, for $\lambda_n(\theta) = (k(\theta))^2$ we have

$$\begin{aligned} \lambda_n &= \theta^2 + V + \frac{V^2}{4\theta} \cot \theta + O(n^{-3/2}), \\ \frac{d\lambda_n}{d\theta} &= 2\theta - \frac{V^2}{4\theta \sin^2 \theta} + O(n^{-5/4}), \\ \frac{d^2 \lambda_n}{d\theta^2} &= 2 + \frac{V^2 \cos \theta}{2\theta \sin^3 \theta} + O(n^{-1}). \end{aligned} \quad (107)$$

Proof. Let us rewrite the formula (103) as

$$k = \theta - V \frac{\sin \theta}{D'(\theta)} \frac{1}{\theta} - \frac{V^2}{2} \left(\frac{\sin \theta}{D'(\theta)} \right)^3 \frac{D''(\theta)}{\theta^2 \sin \theta} + R_3. \quad (108)$$

When θ is in the interval (102), we have

$$\theta = O(n), \quad \theta^{-1} = O(n^{-1}), \quad (\sin \theta)^{-1} = O(n^{1/4}), \quad \cot \theta = O(n^{1/4}). \quad (109)$$

Thus

$$\begin{aligned}
\frac{\sin \theta}{D'(\theta)} &= \frac{\sin \theta}{-2 \sin \theta + V(\theta^{-1} \cos \theta - \theta^{-2} \sin \theta)} \\
&= -\frac{1}{2} \cdot \frac{1}{1 - (V/2)(\theta^{-1} \cot \theta - \theta^{-2})} \\
&= -\frac{1}{2} - \frac{V}{4} \theta^{-1} \cot \theta + O(n^{-3/2}), \\
\left(\frac{\sin \theta}{D'(\theta)} \right)^3 &= -\frac{1}{8} - \frac{3V}{16} \theta^{-1} \cot \theta + O(n^{-3/2}), \\
\frac{D''(\theta)}{\sin \theta} &= \frac{-2 \cos \theta + V(-\theta^{-1} \sin \theta - 2\theta^{-2} \cos \theta + 2\theta^{-3} \sin \theta)}{\sin \theta} \\
&= -2 \cot \theta + O(n^{-1}).
\end{aligned} \tag{110}$$

Thus the first three terms in (108) coincide the formula (106). Let us show that the remainder term R_3 is negligible. By the differentiation of the inverse function, we can prove that

$$(D^{-1})^{(j)}(y) = D'(k)^{-(2j-1)} \cdot (\text{Polynomial of } D'(k), \dots, D^{(j)}(k)). \tag{111}$$

The polynomial part is bounded uniformly with respect to n . By the expansion (76) and the monotonicity of $k = k(\theta)$, we see that $k = k(\theta)$ satisfies

$$(n-1)\pi + \left(\frac{V^2}{4n\pi} \right)^{1/4} + O(n^{-3/4}) \leq k \leq n\pi - \left(\frac{V^2}{4n\pi} \right)^{1/4} + O(n^{-3/4}), \tag{112}$$

and

$$D'(k)^{-1} = (-2 \sin k + O(n^{-1}))^{-1} = O(n^{1/4}). \tag{113}$$

Put $k_z = D^{-1}(D(\theta) - zV \sin \theta / \theta)$ ($0 \leq z \leq 1$), then k_z lies between $k = D^{-1}(2 \cos \theta)$ and $\theta = D^{-1}(D(\theta))$, and by (111)-(113)

$$\begin{aligned}
&(D^{-1})^{(3)} \left(D(\theta) - zV \frac{\sin \theta}{\theta} \right) \\
&= D'(k_z)^{-5} \cdot (\text{Polynomial of } D'(k_z), D''(k_z), D^{(3)}(k_z)) \\
&= O(n^{5/4}).
\end{aligned}$$

Thus, we once have a rough estimate

$$|R_3| = O(n^{-3}) \cdot O(n^{5/4}) = O(n^{-7/4}),$$

so the equation (106) holds with the worse remainder term $O(n^{-7/4})$. However, this conclusion implies

$$|k(\theta) - \theta| = O(n^{-1}), \tag{114}$$

which also implies

$$\begin{aligned}
& (\sin \theta)^3 \cdot (D^{-1})^{(3)} \left(D(\theta) - zV \frac{\sin \theta}{\theta} \right) \\
&= \left(\frac{\sin \theta}{D'(k_z)} \right)^3 \cdot D'(k_z)^{-2} \cdot (\text{Polynomial of } D'(k_z), D''(k_z), D^{(3)}(k_z)) \\
&= O(n^{1/2}),
\end{aligned}$$

Thus we have $|R_3| = O(n^{-5/2})$ and (106) holds.

Other estimates can be obtained by differentiating the formula (103). Then we find the estimate for the remainder term becomes worse by the power $n^{1/4}$ per one differentiation. For example, the leading term in the remainder in (110) is up to constant multiple

$$\theta^{-2} \cot^2 \theta = O(n^{-3/2}).$$

Differentiating this term, we get

$$-2\theta^{-3} \cot^2 \theta + \theta^{-2} \cdot 2 \cot \theta \cdot \left(-\frac{1}{\sin^2 \theta} \right) = O(n^{-5/4}),$$

and the result is worse than $O(n^{-3/2})$ by $n^{1/4}$. As for R_3 ,

$$\begin{aligned}
\frac{dR_3}{d\theta} &= -V^3 \left(\frac{3 \sin^2 \theta \cos \theta}{\theta^3} - \frac{3 \sin^3 \theta}{\theta^4} \right) \int_0^1 \frac{(1-z)^2}{2} (D^{-1})^{(3)} \left(D(\theta) - zV \frac{\sin \theta}{\theta} \right) dz \\
&\quad - V^3 \left(\frac{\sin \theta}{\theta} \right)^3 \int_0^1 \frac{(1-z)^2}{2} (D^{-1})^{(4)} \left(D(\theta) - zV \frac{\sin \theta}{\theta} \right) \\
&\quad \cdot \left(D'(\theta) - zV \left(\frac{\cos \theta}{\theta} - \frac{\sin \theta}{\theta^2} \right) \right) dz. \tag{115}
\end{aligned}$$

For the first term of (115), one $\sin \theta$ in the numerator changed into $\cos \theta$ by differentiation, and the estimate becomes worse by $n^{1/4}$, because of (109). For the second term, that ‘ $(D^{-1})^{(3)}$ ’ turned into $(D^{-1})^{(4)}$ ’, makes two $D'(k_z)$ in the denominator (see (111)), one of which cancels with $D'(\theta)$ appeared next. Thus the estimate also becomes worse by $n^{1/4}$, in total. We can treat the other remainder terms similarly. \square

3.5 Estimate for the amplitude function

We shall give the bound for the amplitude function in (24), that is,

$$\begin{aligned}
a_n(\theta, x, y) &= \Phi_n(\theta, x, y) \frac{dk}{d\theta} \\
&= \frac{-2 \sin k}{D'(k)} \left(\cos kx + \frac{V}{2k} \sin kx \right) \left(\cos ky + \frac{V}{2k} \sin ky \right) \\
&\quad + i \frac{-2 \sin \theta}{D'(k)} \sin k(x-y) + \frac{-2 \sin^2 \theta}{\sin k \cdot D'(k)} \sin kx \sin ky, \tag{116}
\end{aligned}$$

where $x, y \in (0, 1)$ and $k = k(\theta) = D^{-1}(2 \cos \theta)$ given in (47).

Proposition 14. Let $a_n(\theta, x, y)$ given in (116).

(i) The function a_n is bounded uniformly with respect to $\theta \in \mathbf{R}$, $x, y \in (0, 1)$ and $n = 1, 2, \dots$

(ii) Put $\delta_1 = |V|/(n\pi)$, $\delta_2 = (V^2/(4n\pi))^{1/4}$, and

$$\begin{aligned} I_1 &= [(n-1)\pi, (n-1)\pi + \delta_1], & I_2 &= [(n-1)\pi + \delta_1, (n-1)\pi + \delta_2], \\ I_3 &= [(n-1)\pi + \delta_2, n\pi - \delta_2], & I_4 &= [n\pi - \delta_2, n\pi - \delta_1], & I_5 &= [n\pi - \delta_1, n\pi]. \end{aligned}$$

For sufficiently large n , the derivative $a'_n = \partial a_n / \partial \theta$ obeys the following bound

$$|a'_n(\theta, x, y)| \leq \begin{cases} Cn & (\theta \in I_1), \\ C(n^{-1}(\theta - (n-1)\pi)^{-2} + 1) & (\theta \in I_2), \\ C(n^{-1/2} + 1) & (\theta \in I_3), \\ C(n^{-1}(n\pi - \theta)^{-2} + 1) & (\theta \in I_4), \\ Cn & (\theta \in I_5), \end{cases} \quad (117)$$

where C is a positive constant independent of θ , x , y , and n . Especially,

$$\|a'_n\|_{L^1([(n-1)\pi, n\pi])} = \int_{(n-1)\pi}^{n\pi} |a'_n(\theta, x, y)| d\theta$$

is bounded uniformly with respect to n , x , y .

Proof. (i) First we prove $dk/d\theta = -2\sin\theta/D'(k)$ is bounded uniformly with respect to n and $\theta \in [(n-1)\pi, n\pi]$. For $\theta \in I_4 \cup I_5$, we have $\tau = \theta - n\pi = O(n^{-1/4})$, and $h = (-1)^n(y_n - 2\cos\theta) = O(n^{-1/2})$ by (87). Then we have by the expansions (69) and (83)

$$\begin{aligned} k - l_n &= k_- - l_n = -e_1 h^{1/2}(1 + O(n^{-1/2})) = -h^{1/2}(1 + O(n^{-1/2})), \\ D'(k) &= 2d_2(k - l_n)(1 + O(n^{-1/2})) = (-1)^n h^{1/2}(1 + O(n^{-1/2})). \end{aligned} \quad (118)$$

Let $z_n = (-1)^n y_n$ as in (85). Since $z_n \geq 2$,

$$h = z_n - 2\cos\tau \geq 2 - 2\cos\tau = 4\sin^2 \frac{\tau}{2}. \quad (119)$$

Thus

$$\left| \frac{-2\sin\theta}{D'(k)} \right| \leq \left| \frac{2\sin\tau}{2\sin(\tau/2)} \right| (1 + O(n^{-1/2})) = |2\cos(\tau/2)| (1 + O(n^{-1/2})),$$

and the right hand side is uniformly bounded. We can prove $dk/d\theta$ is uniformly bounded for $\theta \in I_1 \cup I_2$ in a similar way. For $\theta \in I_3$, the bounds (109) and (114) hold, so (109) holds even if θ is replaced by k . Then

$$\begin{aligned} \frac{-2\sin\theta}{D'(k)} &= \frac{-2\sin k(1 + O(n^{-1}))}{-2\sin k + V(k^{-1}\cos k - k^{-2}\sin k)} \\ &= \frac{1 + O(n^{-1})}{1 - (V/2)(k^{-1}\cot k - k^{-2})} = 1 + O(n^{-3/4}). \end{aligned} \quad (120)$$

Thus $dk/d\theta$ is uniformly bounded on all the intervals I_1, \dots, I_5 . Similarly we can prove $-2 \sin k / D'(k)$ and $-2 \sin^2 \theta / (\sin k \cdot D'(k))$ are uniformly bounded. The remaining factors are clearly bounded, so we have the conclusion.

(ii) It is sufficient to show the three functions

$$f_1(\theta) = \frac{d}{d\theta} \left(\frac{-2 \sin k}{D'(k)} \right), \quad f_2(\theta) = \frac{d}{d\theta} \left(\frac{-2 \sin \theta}{D'(k)} \right), \quad f_3(\theta) = \frac{d}{d\theta} \left(\frac{-2 \sin^2 \theta}{\sin k \cdot D'(k)} \right)$$

obey the bound (117), since the derivatives of the remaining factors are bounded.

First, by (57), (58) and (25)

$$\begin{aligned} f_1(\theta) &= \frac{-2 \cos k D'(k) + 2 \sin k D''(k)}{D'(k)^2} \cdot \frac{dk}{d\theta} \\ &= \frac{-2 \sin \theta}{D'(k)^3} \cdot V(-2k^{-1} - 2k^{-2} \cos k \sin k + 4k^{-3} \sin^2 k) \\ &= \frac{-2 \sin \theta}{D'(k)^3} \cdot O(n^{-1}). \end{aligned} \tag{121}$$

For $\theta \in I_4 \cup I_5$, the expansion (118) implies

$$\frac{-2 \sin \theta}{D'(k)^3} = -2 \cdot \sin \tau \cdot h^{-3/2} (1 + O(n^{-1/2})). \tag{122}$$

For $\theta \in I_5$, by (86)

$$\begin{aligned} \sin \tau &= O(n^{-1}), \\ h &= z_n - 2 \cos \tau \geq z_n - 2 = \frac{V^2}{4} (n\pi)^{-2} + O(n^{-4}), \quad h^{-3/2} = O(n^3). \end{aligned} \tag{123}$$

Thus (121), (122) and (123) imply $|f_1(\theta)| = O(n)$ for $\theta \in I_5$. For $\theta \in I_4$, we have $|\tau| = O(n^{-1/4})$ and by (119)

$$\begin{aligned} \sin \tau &= \tau(1 + O(n^{-1/2})), \\ h &\geq \tau^2(1 + O(n^{-1/2})), \quad h^{-3/2} \leq \tau^{-3}(1 + O(n^{-1/2})) \end{aligned} \tag{124}$$

for large n . Thus (121), (122) and (124) imply $|f_1(\theta)| \leq Cn^{-1}\tau^{-2}$ for $\theta \in I_4$, for some positive constant C independent of n . For $\theta \in I_3$, we have by (120)

$$-\frac{2 \sin \theta}{D'(k)} = O(1), \quad D'(k)^{-1} = O(n^{1/4}).$$

So (121) implies $|f_1(\theta)| = O(n^{-1/2})$ for $\theta \in I_3$. Similarly we can prove $|f_1(\theta)| = O(n^{-1}(\theta - (n-1)\pi)^{-2})$ for $\theta \in I_2$ and $|f_1(\theta)| = O(n)$ for $\theta \in I_1$, thus $f_1(\theta)$ obeys the bound (117).

Next, we shall estimate $f_2(\theta)$. By (54), (56)-(58) and (25), we have

$$\begin{aligned}
f_2(\theta) &= \frac{-2 \cos \theta \cdot D'(k) + 2 \sin \theta \cdot D''(k) \cdot (-2 \sin \theta)/D'(k)}{D'(k)^2} \\
&= \frac{-D(k)D'(k)^2 - (4 - D(k)^2)D''(k)}{D'(k)^3} \\
&= \frac{1}{D'(k)^3}(-2V^2k^{-2} \cos k + O(n^{-3})) \\
&= \frac{1}{D'(k)^3} \cdot O(n^{-2}).
\end{aligned}$$

This equality and (118), (123), (124) and (109) (with θ replaced by k) gives the same conclusion for $f_2(\theta)$ (actually, we obtain a bit faster decay for $\theta \in I_2 \cup I_3 \cup I_4$).

Finally, by (54), (56)-(58) and (25),

$$\begin{aligned}
\frac{-2 \sin^2 \theta}{\sin k \cdot D'(k)} &= \frac{D(k)^2 - 4}{2 \sin k \cdot D'(k)} = \frac{-4 \sin k + 4Vk^{-1} \cos k + V^2k^{-2} \sin k}{2D'(k)}, \\
f_3(\theta) &= \frac{-2 \sin \theta}{D'(k)^3}(2Vk^{-1} + O(n^{-2})) = \frac{-2 \sin \theta}{D'(k)^3} \cdot O(n^{-1}).
\end{aligned}$$

This estimate is the same as (121). So the same conclusion holds for $f_3(\theta)$. \square

4 Proof of Theorem 1

The $L^1 - L^\infty$ norm of the operator $P_n e^{-itH}$ is just the supremum with respect to $x, y \in \mathbf{R} \setminus \mathbf{Z}$ of the absolute value of the integral kernel $K_{n,t}(x, y)$ given in (24). Put $x = [x] + x'$, $y = [y] + y'$, $[x], [y] \in \mathbf{Z}$, $x', y' \in (0, 1)$, and $s = ([x] - [y])/t$, then (24) is rewritten as⁸

$$K_{n,t}(x, y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-it(\lambda_n(\theta) - s\theta)} a_n(\theta, x', y') d\theta, \quad (125)$$

where a_n is the amplitude function given in (116). The following lemma, taken from Stein's book [15, page 334], gives the decay order of the oscillatory integral with respect to t .

Lemma 15. *Let $I = (a, b)$ be a finite open interval and $k = 1, 2, 3, \dots$. Let $\phi \in C^k(I; \mathbf{R})$, and assume*

$$m_k = \inf_{x \in I} |\phi^{(k)}(x)| > 0.$$

If $k = 1$, we additionally assume ϕ' is a monotone function on I . Let $\psi \in C^1(I; \mathbf{C})$ and assume $\psi' \in L^1(I)$. Then we have

$$\left| \int_a^b e^{it\phi(x)} \psi(x) dx \right| \leq t^{-1/k} \cdot c_k(m_k)^{-1/k} \left(|\psi(b)| + \int_a^b |\psi'(x)| dx \right)$$

for any $t > 0$, where $c_k = 5 \cdot 2^{k-1} - 2$.

⁸This kind of modification is used in the analysis by Korotyaev [8], in which the propagation speed of the wave front in a periodic media is studied.

Remark. Here, we say $f(x)$ is monotone if $f(x) \leq f(y)$ ($x < y$) or $f(x) \geq f(y)$ ($x < y$). The assumption ‘ I is finite’ can be removed if the integral in the left hand side converges. The proof is done by integration by parts and a mathematical induction (see Stein [15, page 332-334]).

Proof of Theorem 1. The statement for $|t| \leq 1$ immediately follows from Proposition 14. By taking the complex conjugate if necessary, we can assume $t > 1$ without loss of generality.

Let θ_0 as in Proposition 11. Let $v_{\max} = |\lambda'_n(\theta_0)|$ be the maximum of the function $|\lambda'_n(\theta)|$. Put $\theta_0 = n\pi + \tau_0$ and $h_0 = (-1)^n(y_n - 2 \cos \theta_0) = z_n - 2 \sin \tau_0$. Put $\delta_n = V^2/(4n\pi)$. Then we have by (99) and (87),

$$\tau_0 = -\delta_n^{1/3} + O(n^{-1}), \quad (126)$$

$$\sin \tau_0 = -\delta_n^{1/3} + O(n^{-1}), \quad (127)$$

$$h_0 = \delta_n^{2/3} + O(n^{-4/3}). \quad (128)$$

Since $\lambda_n(\theta) = \lambda_-(\theta)$ near the upper edge, we have by (126)-(128) and (91)⁹

$$\begin{aligned} v_{\max} &= \lambda'_n(\theta_0) \\ &= 2 \sin \tau_0 \cdot \left(-\frac{1}{2} \lambda_{0,1} h_0^{-1/2} + \lambda_{0,2} - \frac{3}{2} \lambda_{0,3} h_0^{1/2} + 2 \lambda_{0,4} h_0 - \frac{5}{2} \lambda_{0,5} h_0^{3/2} + O(h_0^2) \right) \\ &= 2n\pi (1 + O(n^{-2/3})). \end{aligned} \quad (129)$$

If $|s| \geq v_{\max} + 1$, then we have

$$|\lambda'_n(\theta) - s| \geq |s| - v_{\max} \geq 1. \quad (130)$$

By the periodicity of the integrand, we can divide the integral (125) as the sum of two integrals so that λ'_n is a monotone function on each interval. Then we can apply Lemma 15 with $k = 1$, and we have by (130) and Proposition 14

$$\begin{aligned} |K_{n,t}(x, y)| &\leq 2t^{-1} c_1 \cdot \left(\inf_{\theta \in \mathbf{R}} |\lambda'_n(\theta) - s| \right)^{-1} (\|a\|_{L^\infty(I)} + \|a'\|_{L^1(I)}) \\ &\leq Ct^{-1}, \end{aligned}$$

where $I = [-\pi, \pi]$ and C is a positive constant independent of n .

If $|s| \leq v_{\max} + 1$, then we slide the interval of integration by periodicity, and divide it into four intervals

$$\begin{aligned} I_1 &= [n\pi - 2\delta_n^{1/3}, n\pi - \delta_n^{1/3}/2], \quad I_2 = [n\pi - \delta_n^{1/3}/2, n\pi + \delta_n^{1/3}/2], \\ I_3 &= [n\pi + \delta_n^{1/3}/2, n\pi + 2\delta_n^{1/3}], \quad I_4 = [n\pi + 2\delta_n^{1/3}, (n+2)\pi - 2\delta_n^{1/3}]. \end{aligned}$$

Put

$$K_j = \frac{1}{2\pi} \int_{I_j} e^{-it(\lambda_n(\theta) - s\theta)} a_n(\theta, x', y') d\theta \quad (j = 1, 2, 3, 4).$$

⁹ The formula (129) is consistent with Figure 4.

If $\theta \in I_1$ or I_3 , then $\delta_n^{1/3}/2 \leq |\tau| \leq 2\delta_n^{1/3}$ and by (87)

$$\begin{aligned} h &= \tau^2 + O(\tau^4) + O(n^{-2}) = \tau^2(1 + O(n^{-2/3})), \\ h^{-1} &= \tau^{-2}(1 + O(n^{-2/3})). \end{aligned} \quad (131)$$

By (92),

$$\begin{aligned} \lambda_n''(\theta) &= -2\delta_n h^{-3/2} + 2 + O(n^{-2/3}) \\ &= -2\delta_n |\theta - n\pi|^{-3} + 2 + O(n^{-2/3}) \quad (\theta \in I_1 \cup I_3). \end{aligned} \quad (132)$$

(131) and (132) imply¹⁰

$$\lambda_n''(n\pi \pm 2\delta_n^{1/3}) = \frac{7}{4} + O(n^{-2/3}), \quad (133)$$

$$\lambda_n''(n\pi \pm \delta_n^{1/3}/2) = -14 + O(n^{-2/3}). \quad (134)$$

Next, for $0 < |\tau| < \delta_n^{1/4}$, we have from (87)

$$\frac{V^2}{4}(n\pi)^{-2} + O(n^{-4}) \leq h \leq \tau^2 + O(n^{-1}),$$

and by (97)

$$\lambda_n^{(3)}(\theta) = \sin \tau \cdot \frac{3V^2}{2n\pi} \cdot h^{-5/2} (1 + O(h) + nh^{5/2}O(1)) \neq 0 \quad (0 < |\tau| < \delta_n^{1/4}) \quad (135)$$

for sufficiently large n , since $h = O(n^{-1/2})$ and $nh^{5/2} \cdot O(1) = O(n^{-1/4})$. Thus $\lambda_n^{(2)}$ is monotone on the left half of I_2 . This fact and (134) imply

$$|\lambda_n''(\theta)| \geq |\lambda_n''(n\pi \pm \delta_n^{1/3}/2)| \geq C \quad (\theta \in I_2) \quad (136)$$

for sufficiently large n , for some positive constant C independent of n . Moreover, (133), (135) and (107) imply $|\lambda_n''(\theta)|$ is also uniformly bounded from below on I_4 . Then Lemma 15 implies K_2 and K_4 is $O(t^{-1/2})$, uniformly with respect to n . Moreover, for $\theta \in I_1 \cup I_3$, we have $\delta_n^{1/3}/2 \leq |\tau| \leq 2\delta_n^{1/3}$, and (87) and (135) imply

$$|\lambda_n^{(3)}(\theta)| = 6\delta_n \tau^{-4}(1 + O(\tau^2)) \geq \frac{3}{8}\delta_n^{-1/3}(1 + O(n^{-2/3})) \geq Cn^{1/3} \quad (137)$$

for sufficiently large n , where C is a constant independent of n . Thus Lemma 15 implies

$$|K_1| + |K_3| \leq Ct^{-1/3}n^{-1/9},$$

and the conclusion holds. □

¹⁰ We can make sure the accuracy of the formulas (133) and (134) in Figure 6.

We conclude the paper by arguing the summability of the bandwise estimates. If we fix x, y and take the limit $n \rightarrow \infty$, then $|s| \leq v_{\max}$ for sufficiently large n , by (129) (see also Figure 4). So there always exists the stationary phase point θ_s (the solution to $\lambda'_n(\theta) = s$) nearby $\theta = n\pi$, for sufficiently large n . For simplicity, assume $V > 0$ in the sequel. When $\theta = n\pi$, we have by the formulas (48)-(53), (55), (57) and (58)

$$\begin{aligned} k(n\pi) &= n\pi, \quad k'(n\pi) = k^{(3)}(n\pi) = 0, \\ k''(n\pi) &= D'(n\pi)^{-1}(-2 \cos n\pi) = n\pi(V \cos n\pi)^{-1} \cdot (-2 \cos n\pi) = -\frac{2n\pi}{V}, \\ \lambda'_n(n\pi) &= \lambda_n^{(3)}(n\pi) = 0, \\ \lambda''_n(n\pi) &= 2(k(n\pi)k''(n\pi) + k'(n\pi)^2) = -\frac{4(n\pi)^2}{V}. \end{aligned} \tag{138}$$

Thus, even if we cut out a small interval J_n around $\theta = n\pi$, the bound for the integral over J_n is not better than $O(n^{-1}t^{-1/2})$, which is not summable with respect to n . However, we already know the sum $\sum_{n=1}^{\infty} P_n e^{-itH}$ converges in the strong operator topology in $L^2(\mathbf{R})$. Thus it seems that the sum of the integral kernels converges only conditionally. We have to analyze the cancellation between the integral kernels for two adjacent bands more carefully, in order to obtain a better estimate. We hope to argue this subject in the future.

References

- [1] R. Adami and A. Sacchetti, The transition from diffusion to blow-up for a nonlinear Schrödinger equation in dimension 1, *J. Phys. A: Math. Gen.* **38** (2005), 8379–8392.
- [2] S. Albeverio, F. Gesztesy, R. Høegh-Krohn and H. Holden, *Solvable models in quantum mechanics*, Springer, Berlin, 2nd rev. ed. with an appendix by P. Exner, AMS Chelsea, Providence RI (2005).
- [3] S. Cuccagna, On dispersion for Klein Gordon equation with periodic potential in 1D, *Hokkaido Math. J.* **37** (2008), 627–645.
- [4] F. Gesztesy and W. Kirsch, One-dimensional Schrödinger operators with interactions singular on a discrete set, *J. Reine Angew. Math.* **362**, 28–50 (1985).
- [5] H. Hochstadt, Estimates on the stability intervals for Hill's equation, *Proc. Amer. Math. Soc.* **14**(1963), 930–932.
- [6] A. Jensen and T. Kato, Spectral properties of Schrödinger operators and time decay of the wave functions, *Duke Math.* **46** No. 3 (1979), 583–611.
- [7] W. Kohn, W. Analytic properties of Bloch waves and Wannier functions, *Phys. Rev.* **115** (1959) No. 4, 809–821.

- [8] E. Korotyaev, The propagation of the waves in periodic media at large time, *Asymptotic Analysis* **15** (1997), 1–24.
- [9] H. Kovařík and A. Sacchetti, A nonlinear Schrödinger equation with two symmetric point interactions in one dimension, *J. Phys. A: Math. Theor.* **43** (2010), 155205 (16pp).
- [10] R. Kronig and W. Penney, Quantum Mechanics in Crystal Lattices, *Proc. Royal Soc London* **130** (1931), 499–513.
- [11] J.-L. Journé, A. Soffer, and C. D. Sogge, Decay Estimates for Schrödinger Operators, *Comm. Pure Appl. Math.*, Vol. **XLIV** (1991), 573–604.
- [12] H. Mizutani, Dispersive estimates for Schrödinger equations in dimension one, *RIMS Kôkyûroku Bessatsu* **B16** (2010), 141–151.
- [13] M. Reed and B. Simon, *Methods of modern mathematical physics. I. Functional Analysis*, Academic Press, 1980.
- [14] M. Reed and B. Simon, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press, 1978.
- [15] E. M. Stein, *Harmonic Analysis: Real-Variable Methods, Orthogonality, and Oscillatory Integrals 1st Edition*, Princeton University Press, 1993.
- [16] E. Trubowitz, The inverse problem for periodic potentials, *Comm. Pure Appl. Math.* **30** (1977), no. 3, 321–337.
- [17] K. Yajima, Dispersive Estimates for Schrödinger Equations with Threshold Resonance and Eigenvalue, *Comm. Math. Phys.* **259** (2005), 475–509.
- [18] R. Weder, $L^p - L^{p'}$ Estimates for the Schrödinger Equation on the Line and Inverse Scattering for the Nonlinear Schrödinger Equation with a Potential, *J. Funct. Anal.* **170** (2000), 37–68.

